Fast Inference with Min-Sum Matrix Product

(or how I finished a homework assignment 15 years later)

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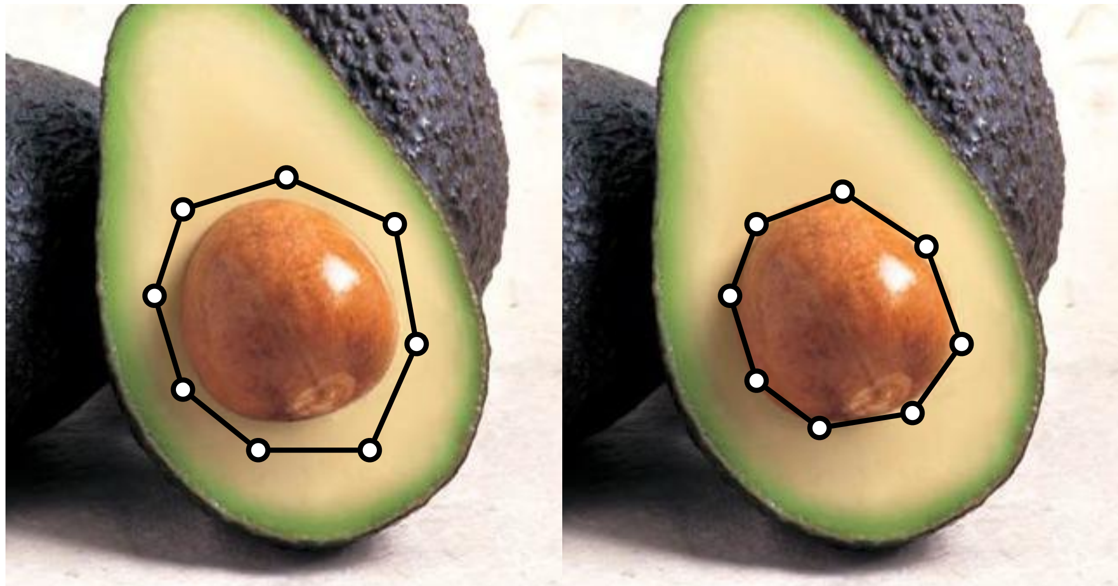
15 years ago, CS664 at Cornell



Active contour models (snakes) for interactive segmentation

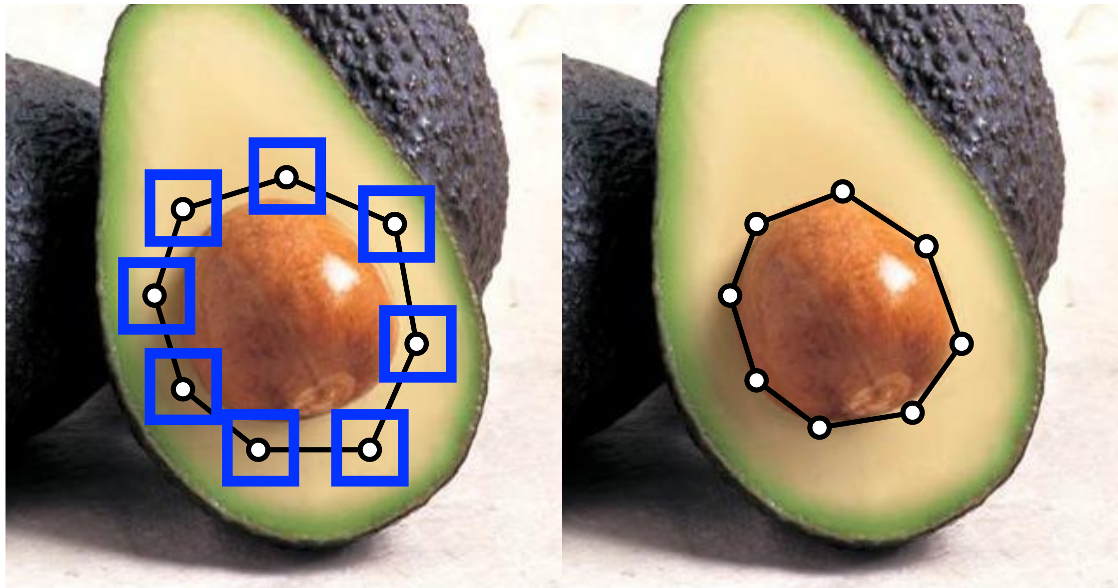
Goal: trace the boundary of an object

User initializes a contour close to an object boundary

Contour moves to the boundary

- Attracted to local features (intensity gradient)
- Internal forces enforce smoothness

Optimization problem



m control points

n possible locations for each point (blue regions)

minimize:

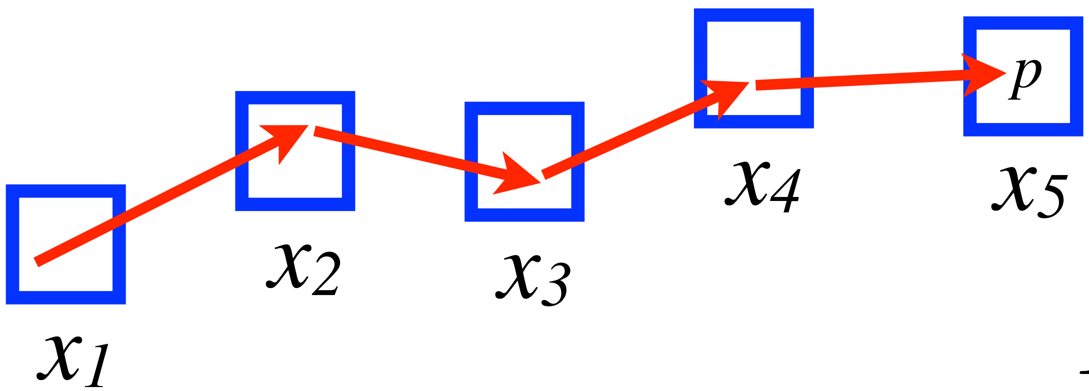
$$E(x_1, \ldots, x_m) = \sum_{i=1}^{m} V_i(x_i, x_{i+1})$$

x_i = location of i-th control point

Many reasonable choices for V

$$V(p, q) = \frac{1}{\text{grad}(I, p, q)} + ||p - q||^2$$

Dynamic programming for open snakes



$$E(x_1, \ldots, x_m) = \sum_{i=1}^{m-1} V_i(x_i, x_{i+1})$$

Shortest path problem

m tables with *n* entries each

$T_i[p]$ = cost of best placement for first *i* points with $x_i = p$

- $T_i[p] = \min_q T_{i-1}[q] + V_i(q, p)$
- Pick best location in T_m, trace-back

$O(mn^2)$ time (optimal in a reasonable sense)

CS664 Homework assignment: Implement closed snakes

pff's solution:

- Consider one control point x_i
- Fixing its location leads to open snake problem
- Try all n possibilities for x_i: $O(mn^3)$ time total

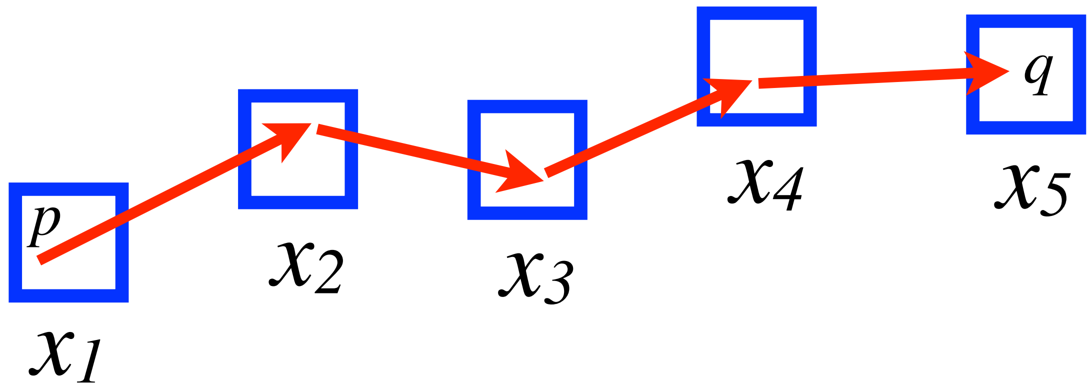
Is this a good solution?

- pff: I think this is the best possible
- rdz: Are you sure?

An alternative solution

Single DP problem

m tables with n^2 entries



$T_i[p, q]$ = cost of best placement for first i points with $x_1 = p$, $x_i = q$

- $T_i[p, q] = \min_r T_{i-1}[p, r] + V_i(r, q)$
- compute T_i from T_{i-1} in $O(n^3)$ time
- Optimal position for x_1 minimizes $T_n[p, p]$
- still $O(mn^3)$ time total...

But, we can write: $T_i = T_{i-1} * V_i$

Min-sum matrix product (MSP), a.k.a. distance product

MSP (min-sum product) / APSP (all-pairs-shortest-paths)

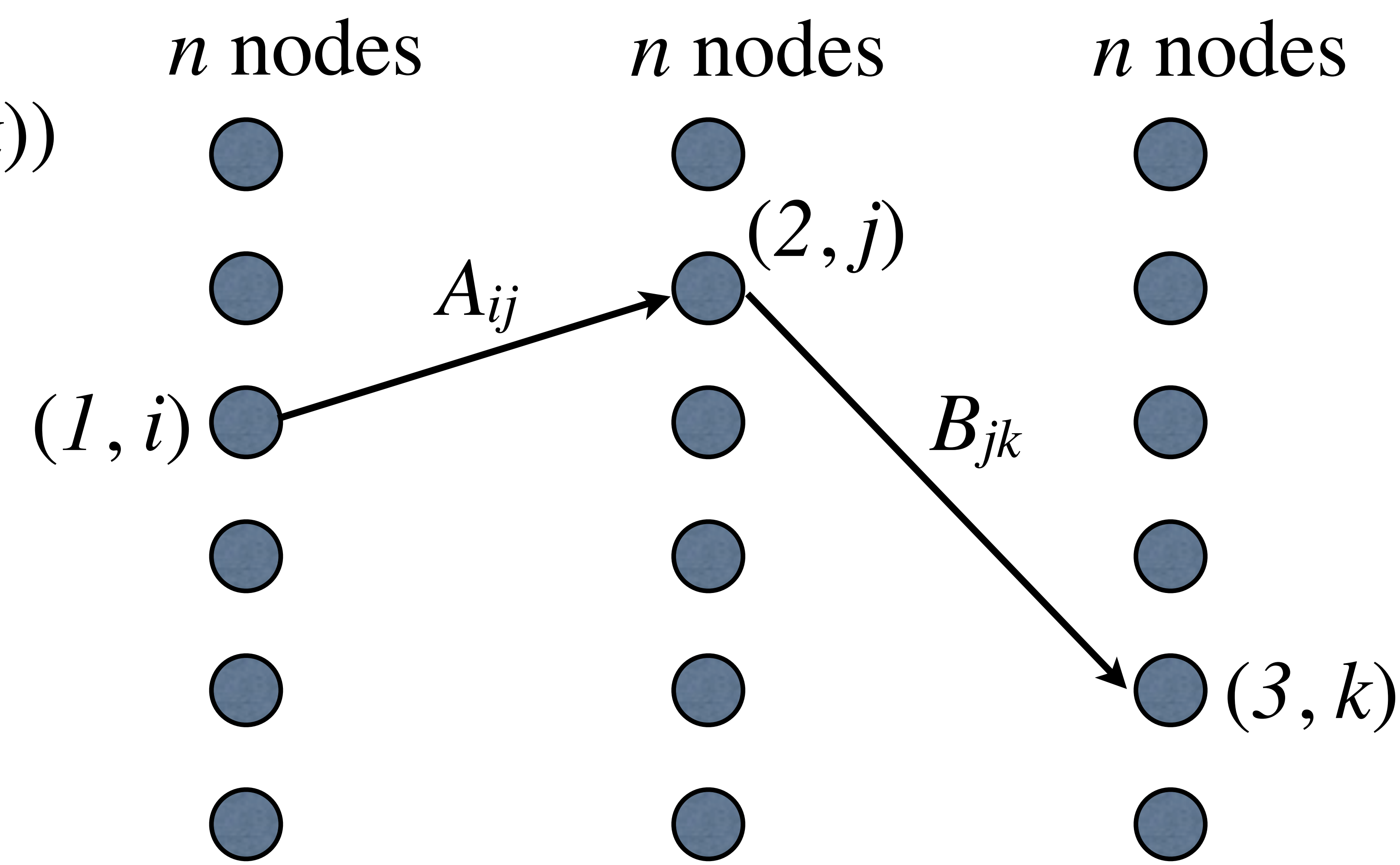
$C = A * B \qquad C_{ik} = \min_j A_{ij} + B_{jk}$

MSP reduces to APSP and vice versa

SP distance matrix in graph with n nodes

$E * E * E * E \ldots = E^n$ (transitive closure of n by n adjacency matrix)

$C_{ik} = \mathrm{d}((1, i), (3, k))$



MSP algorithms

$O(n^3)$ brute force algorithm, $O(n^3 / \log n)$ via APSP

No known algorithm with $O(n^{3-e})$ runtime in the worst case

- Strassen's algorithm doesn't work

Our result: $O(n^2 \log n)$ expected time, assuming values are independent samples from a uniform distribution

With tweaks this really works in practice

- On inputs with significant structure from real applications in vision and natural language

Basic algorithm

MSP(A, B)

$S := \varnothing$
$C_{ik} := \infty$
Initialize Q with entries of A, B, C
while S does not contain all C_{ik} **do**
  $item :=$ remove-min(Q)
  $S := S \cup item$
  if $item = A_{ij}$ **then**
    for $B_{jk} \in S$ relax$(C_{ik}, A_{ij} + B_{jk})$
  end if
  if $item = B_{jk}$ **then**
    for $A_{ij} \in S$ relax$(C_{ik}, A_{ij} + B_{jk})$
  end if
end while

relax(C_{ik}, v)

if $v < C_{ik}$ **then**
  $C_{ik} := v$
  decrease-key(Q, C_{ik})
end if

Correctness

Assume entries in A and B are non-negative

Let $j = \operatorname{argmin} A_{ij} + B_{jk}$

We always have $C_{ik} \geq A_{ij} + B_{jk}$

So A_{ij} and B_{jk} come off the queue before C_{ik}

This implies we call relax$(C_{ik}, A_{ij} + B_{jk})$

When C_{ik} comes off the queue it equals $A_{ij} + B_{jk}$

Implementation

MSP(A, B)

$S := \varnothing$
$C_{ik} := \infty$
Initialize Q with entries of A, B, C
while S does not contain all C_{ik} **do**
  $item :=$ remove-min(Q)
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    for $A_{ij} \in S$ relax$(C_{ik}, A_{ij} + B_{jk})$
  end if
end while

relax(C_{ik}, v)

if $v < C_{ik}$ **then**
  $C_{ik} := v$
  decrease-key(Q, C_{ik})
end if

Maintain $2n$ lists

$I[j]$: list of i such that A_{ij} in S

$K[j]$: list of k such that B_{jk} in S

Running time determined by number of additions and priority queue operations

Runtime Analysis

Let N = # pairs A_{ij}, B_{jk} that are combined before we stop

(both A_{ij}, B_{jk} come off the queue)

- N additions
- $3n^2$ insertions
- at most $3n^2$ remove-min
- at most N decrease-key

Lemma: $E[N] = O(n^2 \log n)$

Using a Fibonacci heap the expected time is $O(n^2 \log n)$

Main lemma

Let N = # pairs A_{ij}, B_{jk} that come off the queue

If entries in A and B are iid samples from a uniform distribution over [0,1] then $E[N] = O(n^2 \log n)$

proof sketch:

Let $X_{ijk} = 1$ if A_{ij} and B_{jk} both come off the queue

$$E[N] = \sum_{ijk} E[X_{ijk}] = \sum_{ijk} P(X_{ijk} = 1).$$

Minimum priority in Q is non-decreasing

Let M be maximum value in C

$X_{ijk} = 1$ if A_{ij} and B_{jk} are at most M

$X_{ijk} = 1$ if A_{ij} and B_{jk} are at most M

The probability that M is large is low

$M \geq \epsilon$ iff one $C_{ik} \geq \epsilon$

$C_{ik} \geq \epsilon$ iff all $A_{ij} + B_{jk} \geq \epsilon$

$P(A_{ij} + B_{jk} \geq \epsilon) = 1 - \epsilon^2/2 \leq e^{-\epsilon^2/2}$

$P(M \geq \epsilon) \leq n^2 e^{-n\epsilon^2/2}$ (union + independence)

The probability that A_{ij} and B_{jk} are both small is low

$P(A_{ij} \leq \epsilon \wedge B_{jk} \leq \epsilon) = \epsilon^2.$

$P(X_{ijk} = 1) \leq n^2 e^{-n\epsilon^2/2} + \epsilon^2.$

Pick $\epsilon = \frac{6 \log n}{n}$

$P(X_{ijk} = 1) \leq \frac{1 + 6 \log n}{n}$

$E[N] \leq n^2(1 + 6 \log n)$

Improvements - normalizing the inputs

1) Subtract min value from each row of A and column of B (add back to C in the end)

2) Remove entries from I/K if we finish a row/column of C

3) (A* search)

Let $a(j)$ be minimum value in column j of A

Let $b(j)$ be minimum value in row j of B

- Put A_{ij} into Q at priority $A_{ij} + b(j)$
- Put B_{jk} into Q at priority $B_{jk} + a(j)$

Practical issues

Fibonacci heap not practical (believe me, we tried)

Practical alternatives:

- Integer queue gives approximation algorithm
- Avoid queue by sorting A and B
  - ok, but not as fast as integer queue
- Scaling method
  - Avoids sorting
  - exact, and fastest in practice

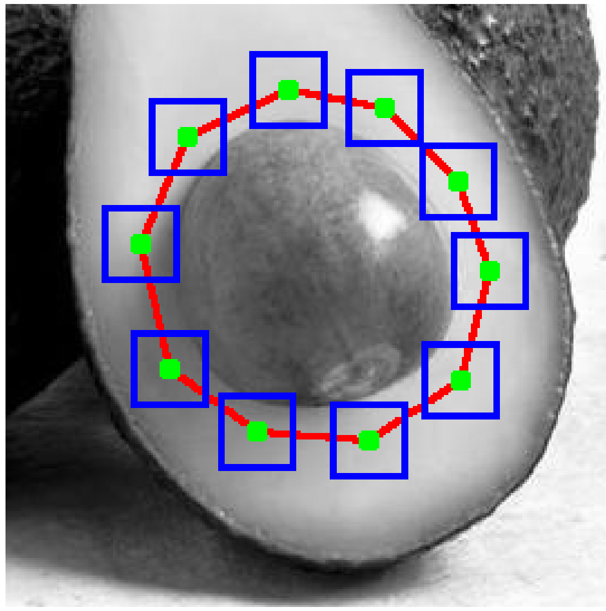
Scaling method

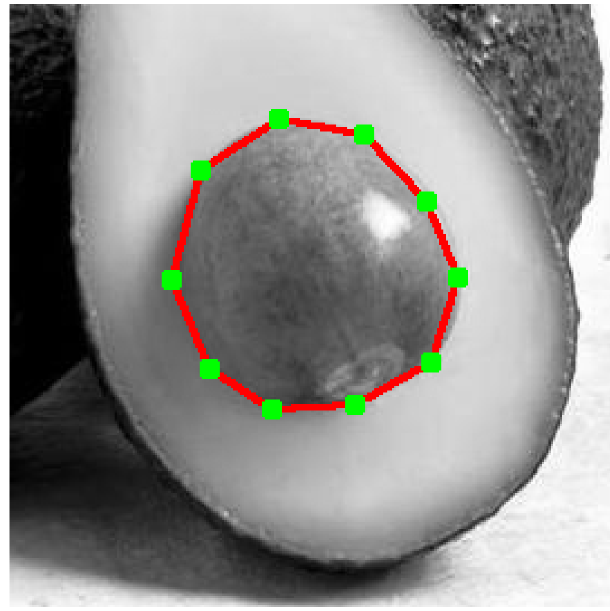
```
C_ik := ∞
T := t-min
while max_ik C_ik > T do
    I[j] := {i | A_ij ≤ T}
    K[j] := {k | B_jk ≤ T}
    for j ∈ {1 ... n} do
        for i ∈ I[j] do
            for k ∈ K[j] do
                C_ik = min(C_ik, A_ij + B_jk)
            end for
        end for
    end for
    T := 2T
end while
```

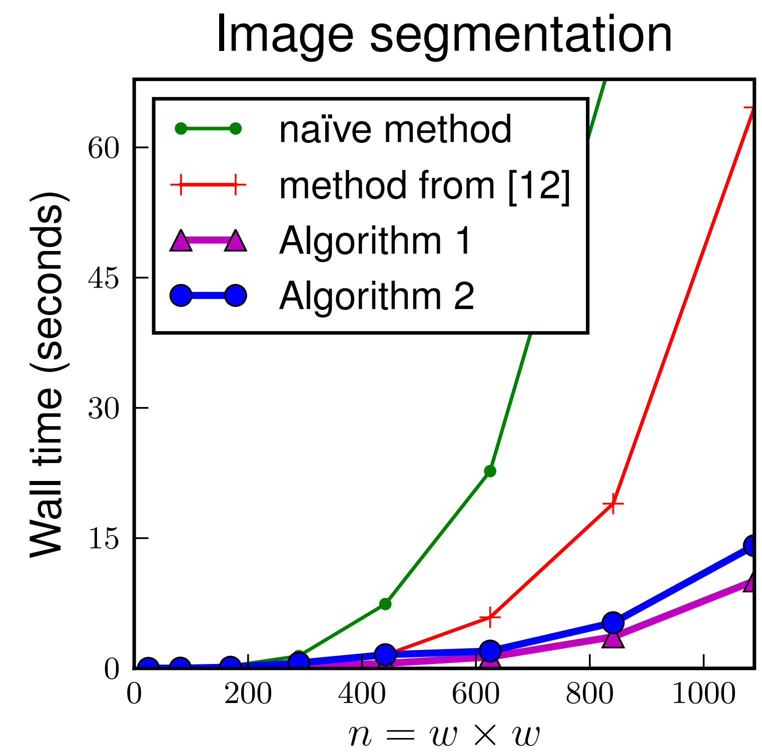
Consider entries of A and B that are at most T

If maximum entry in resulting C is at most T we are done

Experimental results with real data







naive method uses $O(n^3)$ brute-force algorithm MSP

[12] gives an $O(n^{2.5})$ algorithm with (weaker) assumption that entries come in random order

Algorithm 1: integer queue (approximate)

Algorithm 2: scaling method (exact)

Other Applications

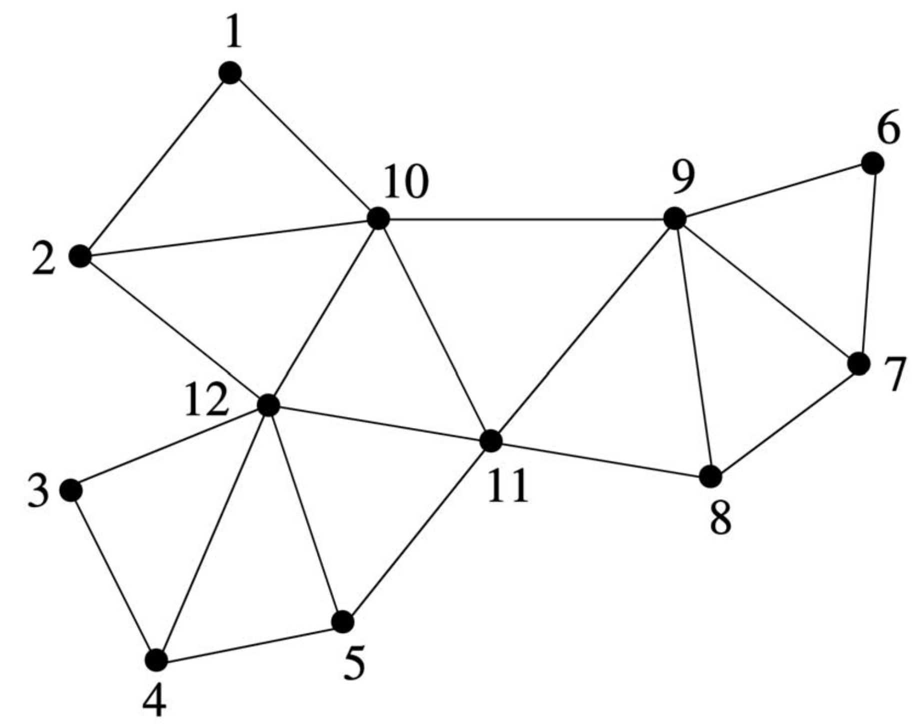
MAP estimation with pairwise graphical model

- m variables, n possible values for each variable

$$E(x_1, \ldots, x_m) = \sum_{i=1}^{m} V_i(x_i) + \sum_{(i,j)\in E} V_{ij}(x_i, x_j)$$

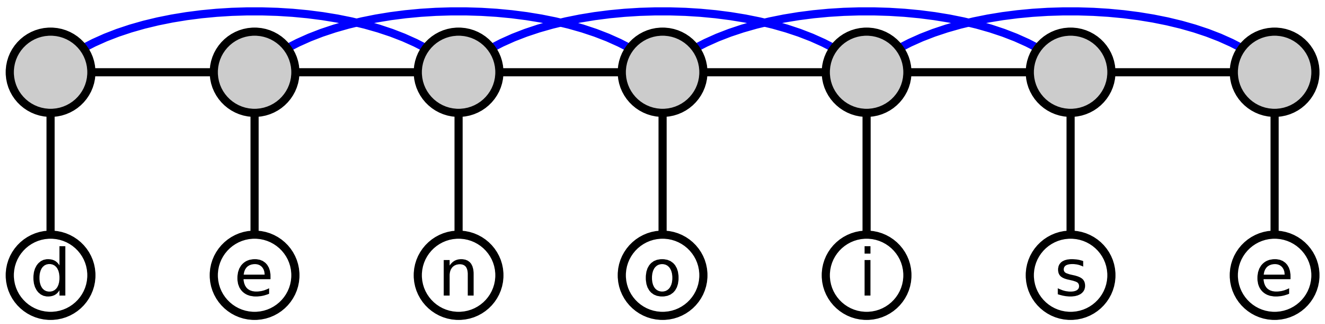
Tree-width 2 model

- m MSP of n by n matrices
- $O(mn^3)$ -> $O(mn^2 \log n)$



Language modeling

Something between bigram and trigram model



- Bigram: $P(x_t \mid x_{t-1})$
- Trigram: $P(x_t \mid x_{t-1}, x_{t-2})$
- Skip-chain: $P(x_t \mid x_{t-1}, x_{t-2}) \sim q_1(x_t, x_{t-1})\, q_2(x_t, x_{t-2})$

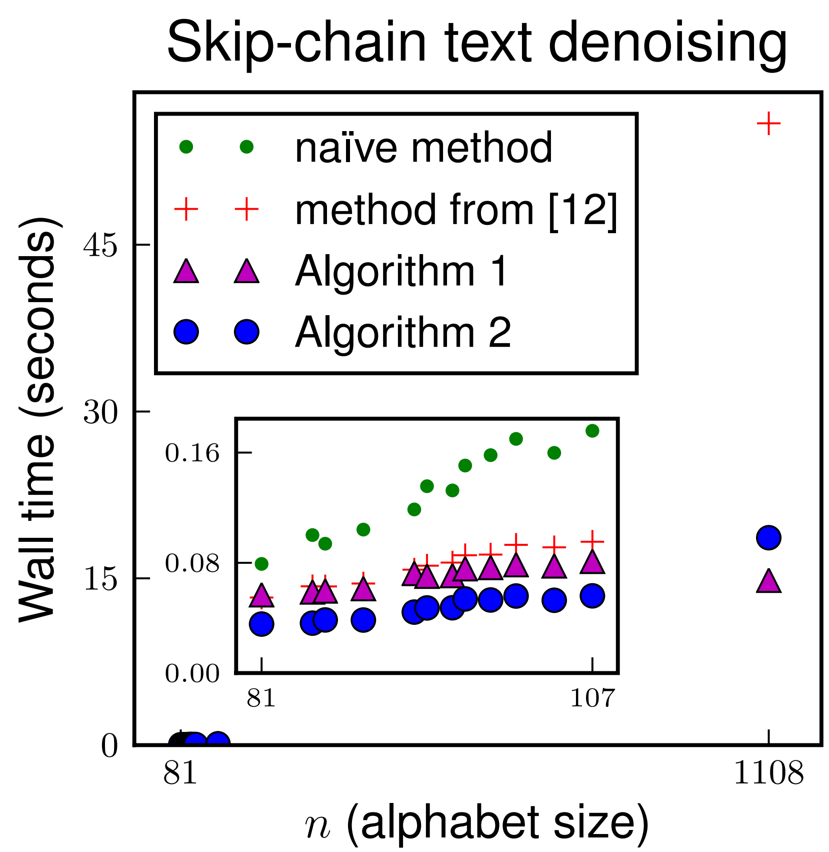
Task: recover a sentence from noisy data

Assume each character is corrupted with probability c

Use skip model as prior over sentences $P(x)$

Given corrupted text y, find x maximizing $P(x|y) \sim P(y|x)P(x)$

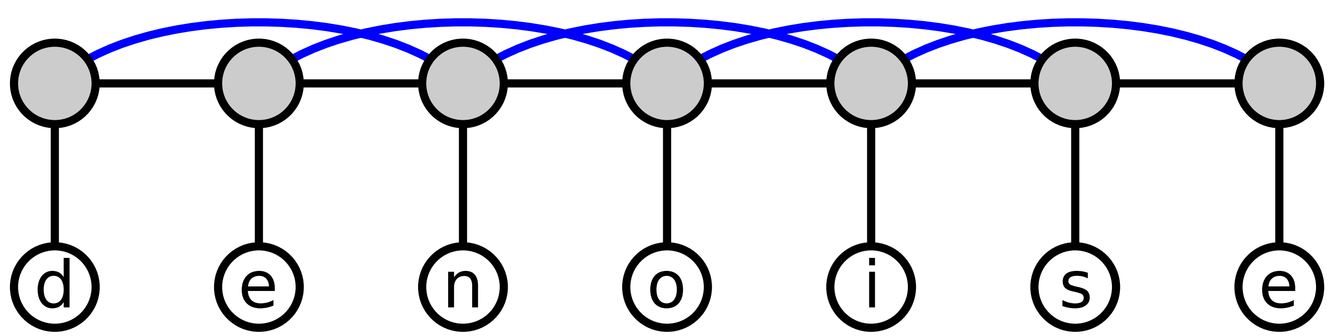
Language modeling



naive method takes $O(mn^3)$

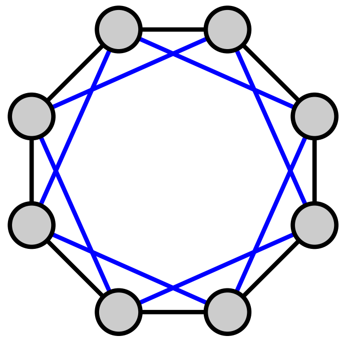
m is the length of the sentence

n is the alphabet size

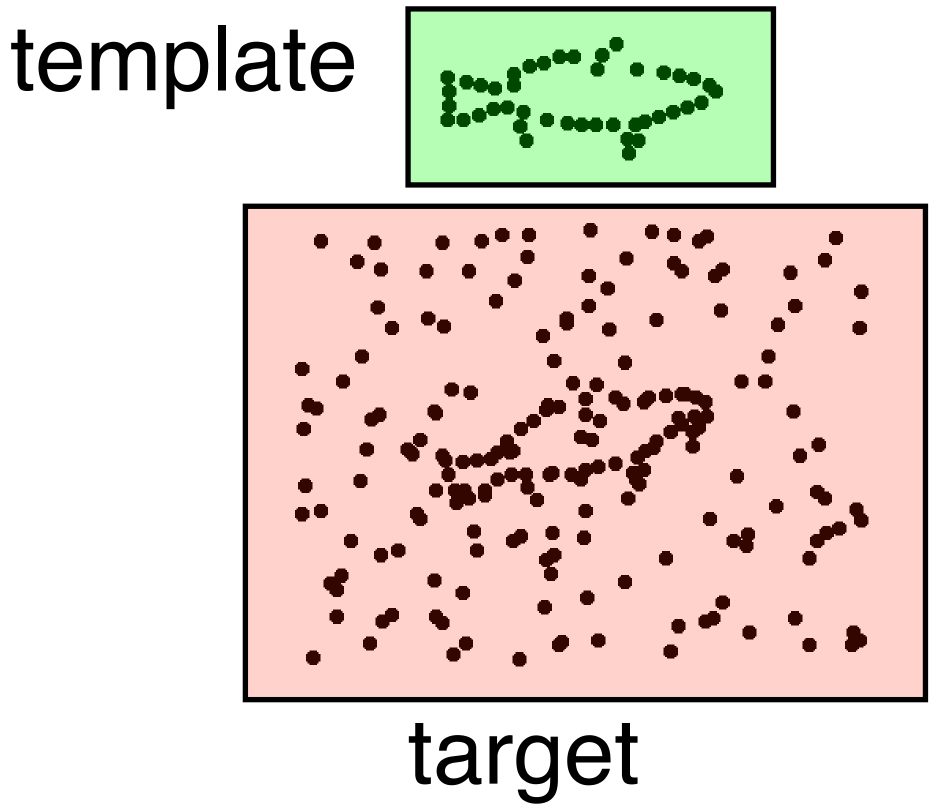


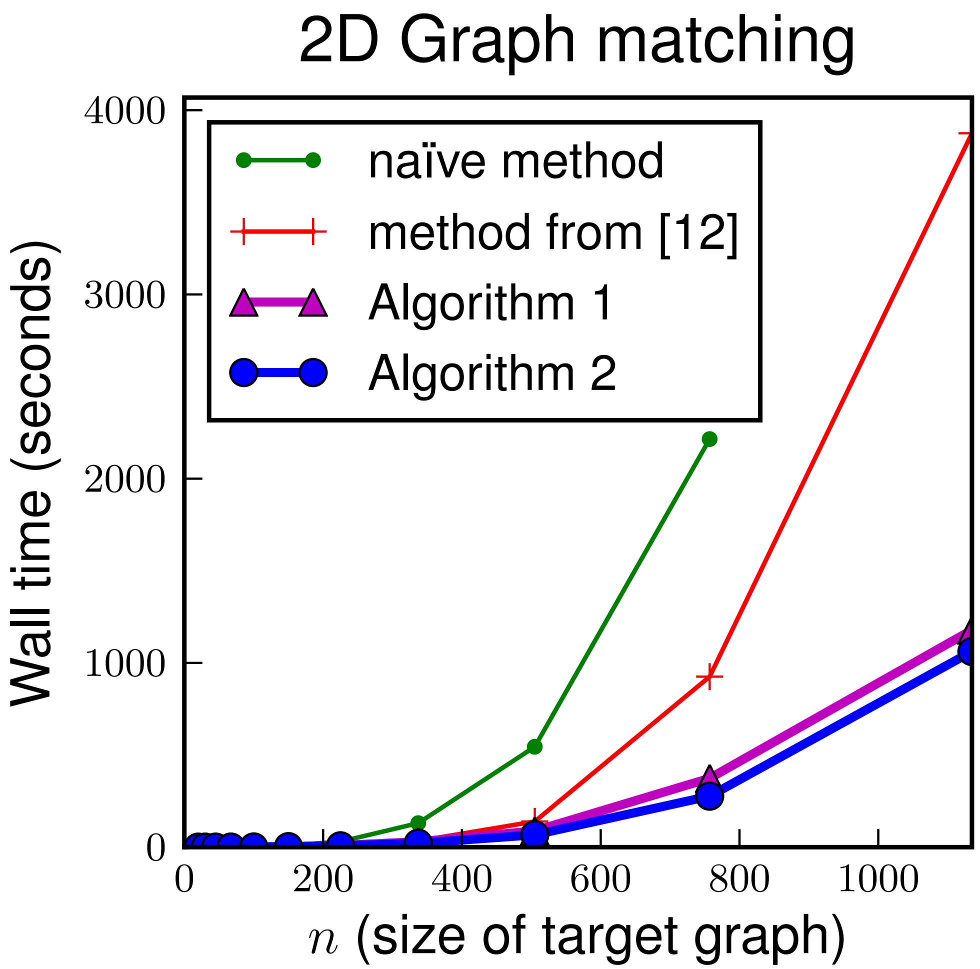
Point pattern matching

Map points in template to points in target preserving distances between certain pairs



(c) Point-matching model





Parsing

Parsing with stochastic context-free grammars

- $O(n^3)$ with dynamic programming (CKY)
- Reduces to MSP with Valiant's transitive closure method

RNA Secondary structure prediction

- $O(n^3)$ dynamic programming
- Reduces to parsing with special grammar

Some open questions

Why does it actually work?

Characterize what “normalization” is doing

How does it relax assumptions on input distribution

$O(n^{3-e})$ worst case (randomized) algorithm for MSP

Can we get a practical parsing method?

Avoid transitive closure machinery?